Data Sheet (Cat.No.T39662)

TargetMol

CCR4 antagonist 3 hydrochloride

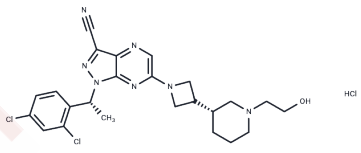
Chemical Properties

CAS No. : 2174938-71-5

Formula: C24H27Cl2N7O.xHCl

Molecular Weight:

Storage: Powder: -20°C for 3 years | In solvent: -80°C for 1 year
Actual storage temperature shall be subject to the COA.



Biological Description

Description	CCR4 antagonist 3 hydrochloride is an orally active, potent and selective CCR4 antagonist. CCR4 antagonist 3, featuring a novel piperidinyl-azetidine motif, has IC 50 s of 22 nM and 50 nM in the calcium flux and CTX assay. CCR4 antagonist 3 has antitumor activity.
Targets(IC50)	Others,CCR
In vitro	CCR4 antagonist 3 (compound 38) shows no activity in a CYP450 induction assay[1]. CCR4 antagonist 3 inhibits the migration of mouse iT reg cells with an IC 50 of 39 nM, while the IC 50 in human iT reg cells is 33 nM[1].
In vivo	CCR4 antagonist 3 (compound 38; 50 mg/kg; PO; daily; for 40 days) significantly reduces tumor growth in six-to-eight-week-old female C57BL/6 mice with Pan02-OVA tumor[1]. CCR4 antagonist 3 demonstrates low clearance (CL=10.2 mL/min/kg), medium volume of distribution (V ss =5.2 L/kg), a half-life (T 1/2) of 6.9 hours, and good bioavailability (%F = 29) in mice at 0.5 mg/kg IV dosing[1]. In dogs, this compound shows low clearance (CL=7.3 mL/min/kg), a half-life of 12.7 hours, and 44% bioavailability, and in cynomolgus monkeys, it exhibits low clearance (CL=3.7 mL/min/kg), a half-life (T 1/2) of 10.7 hours, and 41% bioavailability[1]. In rats, CCR4 antagonist 3 at 0.5 mg/kg IV or 2 mg/kg PO displays medium clearance (CL=47.6 mL/min/kg) and 49% oral bioavailability[1].

Reference

Omar Robles, et al. Novel Piperidinyl-Azetidines as Potent and Selective CCR4 Antagonists Elicit Antitumor Response as Single Agent and in Combination with Checkpoint Inhibitors. J Med Chem. 2020 Jul 15.

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